Mean–Field and Nonlinear Dynamics in Many–Body Quantum Systems

V.R. Manfredi[1,2] and L. Salasnich[2,3]

[1] Dipartimento di Fisica "G. Galilei", Università di Padova,
Via Marzolo 8, I–35131 Padova, Italy
[2] Istituto Nazionale di Fisica Nucleare, Sezione di Padova,
Via Marzolo 8, I–35131 Padova, Italy
[3] Istituto Nazionale per la Fisica della Materia, Unità di Milano,
Dipartimento di Fisica, Università di Milano,
Via Celoria 16, I–20133 Milano, Italy

Abstract. In this paper we discuss in detail the nonlinear equations of the mean–field approximation and their connection to the exact many–body Schrödinger equation. Then we analyze the mean–field approach and the nonlinear dynamics of a trapped condensate of weakly–interacting bosons.

1 Introduction

In the past few years many authors, working in different fields, have shown great interest in the so–called *quantum chaos* or *quantum chaology*, i.e. the signature in the quantal systems of the chaotic properties of the corresponding ($\hbar \to 0$) semiclassical Hamiltonian [1–4]. Incidentally, as stressed by Berry [5], "the semiclassical limit $\hbar \to 0$ and the long time limit $t \to \infty$ are not interchangeable – the origin of the $(\hbar, t^{-1})$ plane is mightily singular".

The subject is very wide but, for reasons of space, we focus our attention only on the connection between the mean–field approximation and the onset of chaos. For a quantum system with discrete spectrum, dynamical chaos is possible only as a transient with lifetime t_H, the so–called Heisenberg time, which scales as the number of degrees of freedom. Because t_H can be very long for a many–body system, we suggest that the *transient chaotic dynamics* of quantum states and the related observables can be experimentally measured. Moreover, when the mean–field theory is a good approximation of the exact many–body problem, one can use the nonlinear mean–field equations to estimate the transient chaotic behaviour of the many–body system. As a specific example, we consider the dynamics of a trapped weakly–interacting Bose–Einstein condensate.

2 Variational principle and mean–field approximation

Let us consider a N–body quantum system with Hamiltonian $\hat{H}$. The exact time–dependent Schrödinger equation can be obtained by imposing the quantum last

action principle on the Dirac action

$$S = \int dt < \psi(t)| i\hbar \frac{\partial}{\partial t} - \hat{H} |\psi(t) > , \tag{1}$$

where ψ is the many–body wavefunction of the system. Looking for stationary points of S with respect to variation of the conjugate wavefunction ψ^* gives

$$i\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi \ . \tag{2}$$

As is well known, it is usually impossible to obtain the exact solution of the many–body Schrödinger equation and some approximation must be used.

In the mean–field approximation the total wavefunction is assumed to be composed of independent particles, i.e. it can be written as a product of single–particle wavefunctions ϕ_j. In the case of identical fermions, ψ must be antisymmetrized [6]. By looking for stationary action with respect to variation of a particular single–particle conjugate wavefunction ϕ_j^* one finds a time–dependent Hartree–Fock equation for each ϕ_j:

$$i\hbar \frac{\partial}{\partial t}\phi_j = \frac{\delta}{\delta \phi_j^*} < \psi|\hat{H}|\psi >= \hat{h}\phi_j \ , \tag{3}$$

where $\hat{h}$ is a one–body operator. The main point is that, in general, the one–body operator $\hat{h}$ is nonlinear. Thus the Hartree–Fock equations are non–linear (integro–)differential equations. These equations can give rise, in some cases, to chaotic behaviour (dynamical chaos) of the mean–field wavefunction.

3 Mean–Field Approximation and Chaos

In the mean–field approximation the mathematical origin of *dynamical chaos* resides in the nonlinearity of the Hartree–Fock equations. These equations provide an approximate description, the best independent–particle description, which describes, for a certain time interval, the very complicated evolution of the true many–body system. Two questions then arise:
1) Does this chaotic behavior persist in time?
2) What is the best physical situation to observe this kind of nonlinearity?

To answer the first question, it should be stressed that quantum systems evolve according to a linear equation and this is an important feature which makes them different from classical systems. Since the Schrödinger equation is linear, so is any of its projections. Its time evolution follows the classical one, including chaotic behaviour, up to t_H. After that, in contrast to the classical dynamics, we get localization (dynamical localization). The Liouville equation, on the other hand, is linear in classical and quantum mechanics. However, for bound systems, the quantum evolution operator has a purely discrete spectrum (therefore no long–term chaotic behaviour). By contrast, the classical evolution operator (Liouville operator) has a continuous spectrum (implying and allowing

chaos). This means that persistent chaotic behaviour in the evolution of the states and observables is not possible. Loosely speaking, chaotic behaviour is possible in quantum mechanics only as a transient with lifetime t_H [7,8].

The Heisenberg time, or break time, can be estimated from the Heisenberg indetermination principle and reads

$$t_H \simeq \frac{\hbar}{\Delta E} \ , \tag{4}$$

where ΔE is the mean energy level spacing and, according to the Thomas-Fermi rule, $\Delta E \propto \hbar^N$, where N is the number of degrees of freedom, i.e. the dimension of the configuration space. So, as $\hbar \to 0$, the Heisenberg time diverges as

$$t_H \sim \hbar^{1-N} \ , \tag{5}$$

and it does so faster, the higher N is [9]. We observe that the limitation to persistent chaotic dynamics in quantum systems does not apply if the spectrum of the Hamiltonian operator $\hat{H}$ is continuous.

Concerning the second question, it is useful to remember that, in the thermodynamic limit, i.e. when the number N of particles tends to infinity at constant density, the spectrum is, in general, continuous and true chaotic phenomena are not excluded [10].

We have seen that the Heisenberg time t_H is very large for systems with many particles. This fact suggests that the *transient chaotic dynamics* of quantum states and observables can be experimentally observed in many–body quantum systems. Moreover, when the mean–field theory is a good approximation of the exact many–body problem, one can use the nonlinear mean–field equations to estimate the properties of the transient chaotic dynamics.

4 Nonlinear dynamics of a Bose condensate

In this section we discuss the mean–field approximation and the nonlinear dynamics for a system of trapped weakly–interacting bosons in the same quantum state, i.e. a Bose–Einstein condensate [11]. In this case the Hartree–Fock equations reduce to only one equation, the Gross-Pitaevskii equation, which describes the dynamics of the condensate [12]. Nowadays, this equation is intensively studied because of the recent experimental achievement of Bose–Einstein condensation for atomic gasses in magnetic traps at very low temperatures (about 10^{-7} Kelvin) [13].

The Hamiltonian operator of a system of N identical bosons of mass m is given by

$$\hat{H} = \sum_{i=1}^{N} \Big(-\frac{\hbar^2}{2m}\nabla_i^2 + V_0(\mathbf{r}_i) \Big) + \frac{1}{2}\sum_{ij=1}^{N} V(\mathbf{r}_i, \mathbf{r}_j) \ , \tag{6}$$

where $V_0(\mathbf{r})$ is an external potential and $V(\mathbf{r},\mathbf{r}')$ is the interaction potential. In the mean-field approximation the totally symmetric many–particle wavefunction of the Bose–Einstein condensate reads

$$\psi(\mathbf{r}_1,...,\mathbf{r}_N,t)=\phi(\mathbf{r}_1,t)...\phi(\mathbf{r}_N,t)\ , \tag{7}$$

where $\phi(\mathbf{r},t)$ is the single particle wavefunction. By using the quantum variational principle for the Dirac action we get the equation

$$i\hbar\frac{\partial}{\partial t}\phi(\mathbf{r},t)=\Big[-\frac{\hbar^2}{2m}\nabla^2+V_0(\mathbf{r})+(N-1)\int d^3\mathbf{r}' V(\mathbf{r},\mathbf{r}')|\phi(\mathbf{r}',t)|^2\Big]\phi(\mathbf{r},t)\ , \tag{8}$$

which is an integro–differential nonlinear Schrödinger equation. If the bosons are weakly interacting, it is possible to substitute the true interaction with a pseudo–potential $V(\mathbf{r},\mathbf{r}')=g\delta^3(\mathbf{r}-\mathbf{r}')$, where $g=4\pi\hbar^2 a_s/m$ is the scattering amplitude and a_s the scattering length. In this way we obtain the so–called Gross–Pitaevskii (GP) equation

$$i\hbar\frac{\partial}{\partial t}\phi(\mathbf{r},t)=\Big[-\frac{\hbar^2}{2m}\nabla^2+V_0(\mathbf{r})+g(N-1)|\phi(\mathbf{r},t)|^2\Big]\phi(\mathbf{r},t)\ . \tag{9}$$

We now consider a triaxially asymmetric harmonic trapping potential of the form

$$V\left(\mathbf{r}\right)=\frac{1}{2}m\omega_0^2\left(\lambda_1^2x^2+\lambda_2^2y^2+\lambda_3^2z^2\right)\ , \tag{10}$$

where λ_i $(i=1,2,3)$ are adimensional constants proportional to the spring constants of the potential along the three axes.

It has been shown, using a hydrodynamical approach [14], that in the strong coupling limit the GP equation has exact solutions which satisfy a set of ordinary differential equations given by

$$\frac{d^2}{d\tau^2}\sigma_i+\lambda_i^2\sigma_i=\frac{\tilde{g}}{\sigma_i\sigma_1\sigma_2\sigma_3}\ , \qquad i=1,2,3\ . \tag{11}$$

These nonlinearly coupled ordinary differential equations describe the time evolution of the widths σ of the condensate wavefunction ψ along each direction [1]. Here, we have defined the coupling constant $\tilde{g}=(2/\pi)^{1/2}(N-1)a_s/a_0$, proportional to the condensate number N and the scattering length a_s. Note that $\tau=\omega_0 t$ and $a_0=(\hbar/m\omega_0)^{1/2}$ is the harmonic oscillator length.

[1] The same equations can be obtained by minimizing the Dirac action S with a trial mean–field wavefunction $\psi(\mathbf{r}_1,...,\mathbf{r}_N,t)=\phi(\mathbf{r}_1,t)...\phi(\mathbf{r}_N,t)$, where

$$\phi\left(\mathbf{r},t\right)=\left(\frac{1}{\pi^3a_0^6\sigma_1^2(t)\sigma_2^2(t)\sigma_3^2(t)}\right)^{1/4}\prod_{i=1,2,3}\exp\left\{-\frac{x_i^2}{2a_0^2\sigma_i^2(t)}+i\beta_i(t)x_i^2\right\}\ ,$$

with $(x_1,x_2,x_3)\equiv(x,y,z)$. σ_i and β_i are the time-dependent variational parameters [15].

The three differential equations correspond to the classical equations of motion for a particle with coordinates σ_i and Hamiltonian

$$H = \frac{1}{2}\left(\dot{\sigma}_1^2 + \dot{\sigma}_2^2 + \dot{\sigma}_3^2\right) + \frac{1}{2}\left(\lambda_1^2\sigma_1^2 + \lambda_2^2\sigma_2^2 + \lambda_3^2\sigma_3^2\right) + \tilde{g}\frac{1}{\sigma_1\sigma_2\sigma_3} \; . \qquad (12)$$

For $\tilde{g} \neq 0$ this Hamiltonian is nonintegrable and thus generic. As is well known, integrable systems are rather exceptional in the sense that they are typically isolated points in the functional space of the Hamiltonians and their measure is zero in this space. If we choose at random a system in nature, the probability that the system is nonintegrable is one [16].

The small oscillations and the nonlinear coupling of these modes have been studied by Dalfovo et al. for $\lambda_1 = \lambda_2 = 1$ and $\lambda_3 = \sqrt{8}$ (axially symmetric trap) [14]. One of us (L.S.) has recently calculated the mode frequencies of the low energy excitations of the condensate in the case of the triaxially asymmetric potential [17]. These excitations correspond to the small oscillations of variables σ's around the equilibrium point, corresponding to the minimum of the effective potential energy of H. The eigenfrequencies ω for the collective motion, in units of ω_0, are found as the solutions of the equation

$$\omega^6 - 3\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2\right)\omega^4 + 8\left(\lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_2^2\lambda_3^2\right)\omega^2 - 20\lambda_1^2\lambda_2^2\lambda_3^2 = 0 \; . \quad (13)$$

Near the minima of the potential the trajectories in the phase–space are quasi–periodic. On the contrary, far from the minima, the effect of the nonlinearity becomes important. As the KAM theorem [18] predicts, parts of phase space become filled with chaotic orbits, while in other parts the toroidal surfaces of the integrable system are deformed but not destroyed. The study of this order–chaos transition for the Bose condensate in the triaxially asymmetric potential is currently under investigation by our group.

5 Conclusions

The main conclusion of this paper is that the use of mean–field approximation leads to nonlinear equations. As a consequence, in some cases, the behaviour of the wavefunctions may be chaotic.

As a specific example, the Bose–Einstein condensation for weakly–interacting trapped bosons has been discussed in great detail.

Acknowledgments

This work has been partially supported by the Ministero dell'Università e della Ricerca Scientifica e Tecnologica (MURST). L.S. thanks INFM for support through a Research Advanced Project on Bose-Einstein Condensation.

References

1. *From Classical to Quantum Chaos*, Conf. Proc. SIF, Ed. by G.F. Dell'Antonio, S. Fantoni and V.R. Manfredi, vol. **41** (Editrice Compositori, Bologna, 1993).
2. M.T. Lopez–Arias, V.R. Manfredi and L. Salasnich, La Rivista del Nuovo Cimento, vol. **17**, n. 5 (1994).
3. *Quantum Chaos*, Proc. of the Int. School "E. Fermi", Course CXIX, Ed. by G. Casati, I. Guarneri and U. Smilansky (North Holland, Amsterdam, 1993).
4. *Quantum Chaos*, Ed. by G. Casati and B. Chirikov (Cambridge Univ. Press, Cambridge, 1995).
5. *Quantum Chaos*, Ed. by H.A. Cerdeira, R. Ramaswamy, M.C. Gutzwiller and G. Casati (World Scientific, Singapore, 1991).
6. A. Fetter and J. Walecka, *Quantum Theory of Many Particle Systems* (McGraw–Hill, New York, 1971).
7. G. Jona–Lasinio, C. Presilla and F. Capasso, Phys. Rev. lett. **68**, 2269 (1992).
8. F. Haake, H. Wiedemann and K. Zyczkowski, Ann. Physik **1**, 531 (1992)
9. M. Robnik, private communication.
10. P. Castiglione, G. Jona-Lasinio and C. Presilla, J. Phys. A **29**, 6169 (1996); G. Jona-Lasinio and C. Presilla, Phys. Rev. Lett. **77**, 4322 (1996).
11. F. Dalfovo, S. Giorgini, L.P. Pitaevskii and S. Stringari, cond-mat/9806038, Rev. Mod. Phys. in press.
12. E.P. Gross, Nuovo Cimento **20**, 454 (1961); L.P. Pitaevskii, Sov. Phys. JEPT **13**, 451 (1961).
13. M. H. Anderson *et al.*, Science **269**, 198 (1995); C. C. Bradley *et al.*, Phys. Rev. Lett. **75**, 1687 (1995); K. B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995).
14. F. Dalfovo, C.Minniti, and L.P. Pitaevskii, Phys. Rev. A **56**, 4855 (1997).
15. L. Salasnich, Mod. Phys. Lett. B **11**, 1249 (1997); L. Salasnich, Mod. Phys. Lett. B **12**, 649 (1998); A. Parola, L. Salasnich and L. Reatto, Phys. Rev. A **57**, R3180 (1998); L. Reatto, A. Parola and L. Salasnich, J. Low Temp. Phys. **113**, n. 3 (1998).
16. M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer–Verlag, New York, 1990); A.J. Lichtenberg and M.A. Lieberman, *Regular and Stochastic Motion*, (Springer–Verlag, New York, 1983).
17. E. Cerboneschi, R. Mannella, E. Arimondo and L. Salasnich, cond-mat/9809371, Phys. Lett. A in press.
18. O. de Almeida, *Hamiltonian Systems: Chaos and Quantization* (Cambridge University Press, Cambridge, 1988).